# Curriculum Vitae of Prof. Marco CATTO

Born October 2nd, 1968.
*Professional address:* Dipartimento di Farmacia-Scienze del Farmaco, Università degli Studi di Bari Aldo Moro, via E. Orabona 4, I-70125 Bari (I).

## *Career:*

*November 2020-*: Associate Professor of Medicinal Chemistry, University of Bari.

*2019-2020*: Researcher at the University of Bari, Department of Pharmacy-Drug Sciences.

*2015-2019*: Associate Professor of Medicinal Chemistry, University of Bari.

*2020*: qualified Full Professor in the National Scientific Qualification procedure.

*2014, 2018*: qualified Associate Professor in the National Scientific Qualification procedure.

*2006-2015:* Researcher at the University of Bari, Department of Pharmacy.

*1995-2006:* graduate research technician at the University of Bari, Department of Pharmacy.

## *Education:*

*January 2004-December 2005:* post-doctoral fellowship in Medicinal Chemistry, University of Bari.

*November 1999-October 2002:* PhD in Medicinal Chemistry, University of Bari; supervisor: prof. A. Carotti.

*April 1995:* degree in Pharmaceutical Chemistry, University of Bari.

## *Research topics and skills:*

- Design of new molecular entities with multitarget activity against neurodegenerative diseases.
- Discovery and/or repurposing of small molecules as antitumor and neuroprotective agents.
- Development and application of biological tests in the screening of small chemical libraries as inhibitors of acetyl- and butyryl-cholinesterase, amyloid aggregation, matrix metalloproteinases, topoisomerases, monoamine oxidases, oxidative stress. Evaluation of pharmacokinetic properties (pKa, brain penetration, solubility).
- Synthesis of biologically active compounds, either through traditional, combinatorial, and multicomponent approaches.
- Application of advanced techniques, such as solid phase support and microwaves, to the organic synthesis.

## *Authoring activity:*

98 articles in peer-reviewed journals;
1 national patent;
1 international patent;
2 book chapters.

Current *h*-index/citations (July 2022): 32/3203 (Scopus); 32/3035 (Web of Science); 36/4032 (Google Scholar).

## *Teaching activity:*

*September 2022:* international member of the examining Jury for MSc thesis “Design and Synthesis of Novel Organic Compounds as Kinase Inhibitors” by Ms. Ghadeer Ashraf Abdallah Mohamed, Faculty of Postgraduate Studies and Scientific Research, German University of Cairo (Egypt).

*July 2022:* international member of the examining Jury for MSc thesis “Development of benzothiophene derivatives as CLK/DYRK inhibitors” by Ms. Yara Ayman Mahmoud, Faculty of Postgraduate Studies and Scientific Research, German University of Cairo (Egypt).

*June 2022:* member of the examining Jury for PhD theses of Doctoral course in Sciences and Technologies of Chemistry and Materials, University of Genoa (Italy).

*September 2021:* international member of the examining Jury for PhD thesis “Design and Synthesis of Multi-Targeted Therapeutic Agents for Neurodegenerative Diseases” by Ms. Donia Eyad, Faculty of Postgraduate Studies and Scientific Research, German University of Cairo (Egypt).

*December 2019:* external examiner for PhD thesis “Synthesis and biological evaluation of nitrogen heterocycle systems as potential antiviral agents” by Ms. Valeria Francesconi, Doctorate course in Sciences and Technologies of Chemistry and Materials, University of Genoa (Italy).

*August 2018 - december 2021:* international co-tutor and member of the examining Jury for PhD thesis “Design, synthesis and characterization of protein-protein interaction disruptors related to early amyloidogenic phenomena in Alzheimer's disease” (Dr. J. Giovannini, University of Caen-Normandy, France) granted by France Alzheimer.

*February 2018:* external examiner for PhD thesis “1,2-Dihydroxy Derivatives as Peptidomimetics of HIV-1 Protease Inhibitors” by Mr. JP Kayembe, 15K4592, Rhodes University (South Africa).

*December 2015:* international member of the examining Jury for PhD thesis “Synthesis of Multitarget Ligands against Alzheimer’s Disease”, University of Rouen (France).

*2020-:* professor of Drug Analysis at the Department of Pharmacy, University of Bari.

*2012-2019:* professor of Pharmaceutical and Toxicological Analysis at the Department of Pharmacy, University of Bari.

*2010-2016:* appointed professor of Drug Analysis at the Faculty of Pharmacy, University of Basilicata.

*2021-2024:* tutor of PhD thesis in Pharmaceutical Sciences (Dr. G. La Spada), University of Bari.

Italian responsible for Erasmus+ agreement (University of Bari/University of Caen-Normandie) and Supervisor of 8 Erasmus+ master theses of outcoming Italian students.

Italian tutor of a Global Thesis project (University of Bari/University of Freiburg) for international co-tutored Master Thesis.

Supervisor of many Master Theses in Pharmacy and Pharmaceutical Chemistry and Technology (University of Bari).

## *Research project/Administration experiences:*

*2021-2023:* Key Area Person for scientific project “BIOMAD”, Horizon Europe Seeds call, University of Bari.

*2021-2023:* Participant to scientific project “GENESI”, University of Bari.

*2019-2021:* participant to PRIN 2017 201744BN5T “Novel anticancer agents endowed with multi-targeting mechanism of action”.

*2017:* grantee of FFABR funding (Italian Ministry of University and Research.)

*2015-2017:* Participant to scientific project “Cluster in Bioimaging”, University of Bari.

*2008-2010:* participant to PRIN 2008 “Progettazione, sintesi e valutazione biofarmacologica di nuove molecole multipotenti per il trattamento di malattie neurodegenerative rare (morbo di Hungtington e Sclerosi Laterale Amiotrofica)”.

### *International research experiences:*

*July 2015, July 2016:* visiting professor at the CERMN - University of Caen-Normandie (France).

*July-September 2013:* visiting researcher at the University of Geneva-Lausanne (Swiss), research group of prof. P.-A. Carrupt.

*June-October 2002:* guest researcher at the University of Heidelberg (D), research group of prof. T. J. J. Müller.

### *Editorial activities:*

*2019:* Guest co-Editor for Molecules, special issue “Indole and Its Bioisosteric Replacements in Medicinal Chemistry”.

### *Conference presentations:*

*September 2021:* oral communication at *XXVII National Congress of Italian Chemical Society*, FAR-OR031, Book of Abstract p. 134, September 14-23, 2021 (Milan, I; virtual mode); ISBN 978-88-94952-24-7.

*May 2019:* oral communication at *2nd Molecules Medicinal Chemistry Symposium (MMCS 2019),* Book of Abstract p. 134, May 15-17, 2019 (Barcelona, SP).

*July 2018:* oral communication at *Italian-Spanish-Portuguese Joint Meeting in Medicinal Chemistry (MedChemSicily2018),*SC-10, Book of Abstract p. 56, July 17-20, 2018 (Palermo, I).

*September 2013:* invited speaker at *XXVIII Seminar of Pharmaceutical Sciences* of Ecole de Pharmacie Genève-Lausanne (Zermatt, CH).

*July 2009:* oral communication at *XXIII National Congress of Italian Chemical Society* (Sorrento, I).

*February 2004:* oral communication at *Cofin 2002 – Design and Synthesis of Neuroprotective Agents* (Parma, I).

*June 2001:* oral communication at *Cofin 2000 – Design and Synthesis of Neuroprotective Agents* (Genoa, I).

### *Other conferences and courses attended:*

*September 2022:* member of Scientific Secretariat and session Chairperson of *XXVII National Meeting in Medicinal Chemistry (NMMC27)*, September 11 – 14, 2022 (Bari, I).

*October 2021:* participation to 5fth ERNEST Meeting COST Action CA18133, Bridging Perspectives and Networking in Signal Transduction Research, October 4 – 8, 2021 (Bari, I).

*July 2019:* participation (with poster presentation) to *XXVI National Meeting in Medicinal Chemistry (NMMC 2019)* (Milan, I).

*June 2019:* participation to *Paul Ehrlich Euro-PhD Network & MuTaLig COST Action meeting (MedChem2019)* (Catanzaro, I).

*July 2016:* participation to *52nd edition of the International Conference on Medicinal Chemistry (RICT 2016)* (Caen, F).

*September 2011:* participation to *Summer Course on Pharmaceutical Analysis 2011* (Pavia, I).

*May 2010:* participation to *I IDDI Workshop in Neglected and Orphan Diseases* (Siena, I).

*September 2009:* participation to *14th Summer Course on Pharmaceutical Analysis* (Milan, I).

*February 2009:* participation to 3rd meeting-workshop *New Perspectives in Pharmaceutical Chemistry* (University of Pisa, I).

*September 2008:* participation to *13th Summer Course on Pharmaceutical Analysis* (Rimini, I).

*October 2007:* participation to *Frontiers in CNS and Oncology Medicinal Chemistry* (Siena, I).

*March 2006:* participation to *EMBO-FEBS Workshop on Amyloid Formation*, (Florence, I).

*October 2005:* participation to *Quo vadis, Proteomics?*, 2nd International Workshop on the Prospects of Proteomics (Naples, I).

*July 2004:* participation to *XXIV Advanced Course in Medicinal Chemistry* (University of Urbino, I).

*February 2004:* participation to *3rd Laboratory of Synthetic Methodologies in Pharmaceutical Chemistry* (University of Siena, I).

*April 2003:* participation to *2nd International Conference on Multicomponent Reactions, Combinatorial and Related Chemistry* (Genoa, I).

*December 2001:* participation to *Course of Mass Spectrometry for the Study of Proteins and Oligonucleotides* (University of Tuscia, I).

*November 2001:* participation to *1st Laboratory of Synthetic Methodologies in Pharmaceutical Chemistry* (University of Siena, I).

*September 2001:* participation to *II Course in Mass Spectrometry in the Science of Materials* (Padua, I).

*July 2001:* participation to *XXI Advanced Course in Medicinal Chemistry* (University of Urbino, I).

*July 2000:* participation to *XX Advanced Course in Medicinal Chemistry* (University of Urbino, I).

*March 2000:* participation to *4th Course of Mass Spectrometry for PhD students* (University of Siena, I).

### *Peer reviewing/refereeing activities:*

*2015:* External reviewer of grant application for Ligue Européenne contre la Maladie d'Alzheimer (LECMA).

*2013:* External reviewer for Italian Ministry for University and Research (MIUR) in research grant applications.

Peer reviewer for the following journals: ACS Chemical Neurosciences, ACS Medicinal Chemistry Letters, ACS Omega, Amino Acids, Archiv der Pharmazie, BBA - Proteins and Proteomics, Bioorganic Chemistry, Bioorganic and Medicinal Chemistry, Bioorganic and Medicinal Chemistry Letters, Chemical Biology and Drug Design,

ChemBioChem, Chemistry–A European Journal, Chemistry and Biodiversity, ChemistrySelect, Current Pharmaceutical Design, European Journal of Medicinal Chemistry, European Journal of Pharmaceutical Sciences, European Polymer Journal, Expert Opinion On Drug Discovery, Expert Opinion On Drug Metabolism & Toxicology, Future Medicinal Chemistry, International Journal of Molecular Sciences, Journal of Applied Biomedicine, Journal of Enzyme Inhibition and Medicinal Chemistry, Journal of Functional Foods, Journal of Medicinal Chemistry, Letters in Drug Design and Discovery, Molecular and Cellular Probes, Molecules, Monatshefte für Chemie.

### *Professional memberships:*

- Teachers' board of Doctoral School of Pharmaceutical Sciences (University of Bari), 2019-.
- Italian Chemical Society, Medicinal Chemistry Division.

## Articles

1) Altomare C, Cellamare S, Summo L, Catto M, Carotti A, Thull U, Carrupt PA, Testa B, Stoeckli-Evans H; **Inhibition of Monoamine Oxidase-B by Condensed Pyridazines and Pyrimidines: Effects of Lipophilicity and Structure-Activity Relationships.** *J. Med. Chem.* **1998**, 41, 3812-3820.

2) Gnerre C, Catto M, Leonetti F, Weber P, Carrupt PA, Altomare C, Carotti A, Testa B; **Inhibition of Monoamine Oxidases by Functionalised Coumarin Derivatives: Biological Activities, QSARs, and 3D-QSARs.** *J. Med. Chem.* **2000**, 43, 4747-4758.

3) Brühlmann C, Ooms F, Carrupt PA, Testa B, Catto M, Leonetti F, Altomare C, Carotti A; **Coumarin Derivatives as Dual Inhibitors of Acetylcholinesterase and Monoamine Oxidase.** *J. Med. Chem.* **2001**, 44, 3195-3198.

4) Voskressensky LG, Borisova TN, Kulikova LN, Varlamov AV, Catto M, Altomare C, Carotti A; **Tandem Cleavage of Hydrogenated β- and γ-Carbolines. New Practical Synthesis of Tetrahydroazocino[4,5-b]indoles and Tetrahydroazocino[5,4-b]indoles Showing Acetylcholinesterase Inhibitory Activity.** *Eur. J. Org. Chem.* **2004**, 3128-3135.

5) Bachman KE, Sager J, Cheong I, Catto M, Bardelli A, Park BH, Vogelstein B, Carotti A, Kinzler KW, Lengauer C; **Identification of compounds that inhibit growth of 2-amino-1-methyl-6-phenylimidazo(4,5-b)pyridine-resistant cancer cells.** *Mol. Cancer Ther.* **2005**, 4, 1026-1030.

6) Novaroli L, Reist M, Favre E, Carotti A, Catto M, Carrupt P-A; **Human recombinant monoamine oxidase B as reliable and efficient enzyme source for inhibitor screening.** *Bioorg. Med. Chem.* **2005**, 13, 6212-6217.

7) Carotti A, Leonetti F, Stefanachi A, Catto M, Capaldi C, Muncipinto G, Pisani L, Nicolotti O; **In silico design and microwave-assisted solid phase synthesis of focused libraries of enzyme inhibitors with potential in cancer and neurological therapies.** *Sci. Pharm.* **2005**, 13, S 27.

8) Carotti A, Altomare C, Catto M, Gnerre C, Summo L, De Marco A, Rose S, Jenner P, Testa B; **Lipophilicity Plays a Major Role in Modulating the Inhibition of Monoamine Oxidase B by 7-Substituted Coumarins.** *Chem.Biodiv.* **2006**, 3, 134-149.

9) Catto M, Nicolotti O, Leonetti F, Carotti A, Favia AD, Soto-Otero R, Méndez-Álvarez E, Carotti A; **Structural Insights into MAO Inhibitory Potency and Selectivity of 7-substituted Coumarins from Ligand- and Target-based Approaches.** *J. Med. Chem.* **2006**, 49, 4912-4925.

10) Carotti A, De Candia M, Catto M, Borisova TN, Varlamov AV, Méndez-Álvarez E, Soto-Otero R, Voskressensky LG, Altomare C; **Ester Derivatives of Annulated Tetrahydroazocines: a New Class of Selective Acetylcholinesterase Inhibitors.** *Bioorg. Med. Chem.* **2006**, 14, 7205-7212.

11) Novaroli L, Daina A, Favre E, Bravo J, Carotti A, Leonetti F, Catto M, Carrupt P-A, Reist M; **Impact of Species-Dependent Differences on Screening, Design, and Development of MAO B Inhibitors.** *J. Med. Chem.* **2006**, 49, 6264-6272.

12) Carotti A, Catto M, Leonetti F, Campagna F, Soto-Otero R, Méndez-Álvarez E, Thull U, Testa B, Altomare C; **Synthesis and Monoamine Oxidase Inhibitory Activity of New Pyridazine-,Pyrimidine- and 1,2,4-Triazine-Containing Tricyclic Derivatives**. *J. Med. Chem.* **2007**, 50, 5364-5371.

13) Cellamare S, Stefanachi A, Stolfa DA, Basile T, Catto M, Campagna F, Sotelo E, Acquafredda P, Carotti A; **Design, synthesis, and biological evaluation of glycine-based molecular tongs as inhibitors of $A\beta_{1-40}$ aggregation in vitro.** *Bioorg. Med. Chem.* **2008**, 16, 4810-4822.

14) Leonetti F, Catto M, Nicolotti O, Pisani L, Cappa A, Stefanachi A, Carotti A; **Homo- and Hetero-bivalent Edrophonium-like Ammonium Salts as Highly Potent, Dual Binding Site AChE Inhibitors.** *Bioorg. Med. Chem.* **2008**, 16, 7450-7456.

15) Colombo R, Carotti A, Catto M, Racchi M, Lanni C, Verga L, Caccialanza G, De Lorenzi E; **Capillary Electrophoresis Can Identify Small Molecules that Selectively Target Soluble Oligomers of Aβ−protein and Display Antifibrillogenic Activity.** *Electrophoresis* **2009**, 30, 1418-1429.

16) Convertino M, Pellarin R, Catto M, Carotti A, Caflisch A; **9,10-Anthraquinone hinders β-aggregation: how does a small molecule interfere with Aβ-peptide amyloid fibrillation?** *Prot. Sci.* **2009**, 18, 792-800.

17) Pisani L, Muncipinto G, Miscioscia TF, Nicolotti O, Leonetti F, Catto M, Caccia C, Salvati P, Soto-Otero R, Mendez-Alvarez E, Passeleu C, Carotti A; **Discovery of a Novel Class of Potent Coumarin MAO-B inhibitors: Development and Biopharmacological Profiling of 7-[(3-Chlorobenzyl)oxy]-4-[(methylamino)methyl]-2*H*-chromen-2-one methanesulfonate (NW-1772) as a Highly Potent, Selective, Reversible and Orally Active MAO-B inhibitor.** *J. Med. Chem.* **2009**, 52, 6685–6706.

18) Catto M, Aliano R, Carotti A, Cellamare S, Palluotto F, Purgatorio R, De Stradis A, Campagna F; **Design, synthesis and biological evaluation of indane- 2-arylhydrazinylmethylene-1,3-diones and indol-2-aryldiazenylmethylene-3-ones as β-amyloid aggregation inhibitors.** *Eur. J. Med. Chem.* **2010**, 45, 1359-1366.

19) Pellegrino G, Leonetti F, Carotti A, Nicolotti O, Pisani L, Stefanachi A, Catto M; **Solid phase synthesis of a molecular library of pyrimidines, pyrazoles and isoxazoles with biological potential.** *Tetr. Lett.* **2010**, 51, 1702-1705.

20) Pisani L, Catto M, Giangreco I, Leonetti F, Nicolotti O, Stefanachi A, Cellamare S, Carotti A; **Design, Synthesis and Biological Evaluation of Coumarin Derivatives Tethered to an Edrophonium-like Fragment as Highly Potent and Selective Dual Binding Site Acetylcholinesterase Inhibitors.** *Chem. Med. Chem.* **2010**, 5, 1616-1630.

21) Campagna F, Catto M, Purgatorio R, Altomare CD, Carotti A, De Stradis A, Palazzo G; **Synthesis and biophysical evaluation of arylhydrazono-1H-2-indolinones as β-amyloid aggregation inhibitors**. *Eur. J. Med. Chem.* **2011**, 46, 275-284.

22) Nicolotti O, Pisani L, Catto M, Leonetti F, Giangreco I, Stefanachi A, Carotti A; **Discovery of a potent and selective hetero-bivalent AChE inhibitor via bioisosteric replacement.** *Mol. Inform.* **2011**, 30, 133-136.

23) Stefanachi A, Favia AD, Nicolotti O, Leonetti F, Pisani L, Catto M, Zimmer C, Hartmann RW, Carotti A; **Design, Synthesis, and Biological Evaluation of Imidazolyl Derivatives of 4,7-Disubstituted Coumarins as Aromatase Inhibitors Selective over 17-alphahydroxylase/C17-20 lyase.** *J. Med. Chem.* **2011**, 54, 1613-1625.

24) Tasso B, Catto M, Nicolotti O, Novelli F, Tonelli M, Giangreco I, Pisani L, Sparatore A, Boido V, Carotti A, Sparatore F; **Quinolizidinyl Derivatives of Bi- and Tricyclic Systems as Potent Inhibitors of Acetyl- and Butyrylcholinesterase with Potential in Alzheimer's Disease.** *Eur. J. Med. Chem.* **2011**, 46, 2170-2184.

25) Conejo-García A, Pisani L, del Carmen Núñez M, Catto M, Nicolotti O, Leonetti F, Campos J, Gallo M, Espinosa A, Carotti A; **Homodimeric bis-Quaternary Heterocyclic Ammonium Salts as Potent Acetyl- and Butyrylcholinesterase Inhibitors: A Systematic Investigation of the Influence of Linker and Cationic Heads Over Affinity and Selectivity.** *J. Med. Chem.* **2011**, 54, 2627-2645.

26) Leonetti F, Stefanachi A, Nicolotti O, Catto M, Pisani L, Cellamare S, Carotti A; **BCR-ABL Inhibitors in Chronic Myeloid Leukemia: Process Chemistry and Biopharmacological Profile.** *Curr. Med. Chem.* **2011**, 18, 2943-2959.

27) Pisani L, Catto M, Leonetti F, Nicolotti O, Stefanachi A, Campagna F, Carotti A; **Targeting Monoamine Oxidases with Multipotent Ligands: An Emerging Strategy in the Search of New Drugs Against Neurodegenerative Diseases.** *Curr. Med. Chem.* **2011**, 18, 4568-4587.

28) Giangreco I, Lattanzi G, Nicolotti O, Catto M, Laghezza A, Leonetti F, Stefanachi A, Carotti A; **Insights into the complex formed by Matrix Metalloproteinase-2 and alloxan inhibitors: molecular dynamics simulations and free energy calculations.** *PLoS One* **2011**, 6, e25597.

29) Nicolotti O, Convertino M, Leonetti F, Catto M, Cellamare S, Carotti A; **Estimation of the Binding Free Energy by Linear Interaction Energy Models**. *Mini Rev. Med. Chem.* **2012**, 12, 551-561.

30) Stefanachi A, Leonetti F, Nicolotti O, Catto M, Pisani L, Cellamare S, Altomare C, Carotti A; **New Strategies in the Chemotherapy of Leukemia: Eradicating Cancer Stem Cells in Chronic Myeloid Leukemia.** *Curr. Cancer Drug Targets*, **2012**, 12, 571-596.

31) Leonetti F, Muncipinto G, Stefanachi A, Nicolotti O, Cellamare S, Catto M, Pisani L, Pellegrino G, Carotti A; **Towards a fragment-based approach to MMPs inhibitors: an expedite and efficient synthesis of N-hydroxylactams.** *Tetr. Lett.* **2012**, 53, 4114-4116.

32) Oppedisano F, Catto M, Koutentis PA, Nicolotti O, Pochini L, Koyioni M, Introcaso A, Michaelidou SS, Carotti A, Indiveri C; **Inactivation of the glutamine/amino acid transporter ASCT2 by 1,2,3-dithiazoles: Proteoliposomes as a tool to gain insights in the molecular mechanism of action and of antitumour activity.** *Toxicol. Appl. Pharmacol.* **2012**, 265, 93-102.

33) Nicolotti O, Catto M, Giangreco I, Barletta M, Leonetti F, Stefanachi A, Pisani L, Cellamare S, Tortorella P, Loiodice F, Carotti A; **Design, synthesis and biological evaluation of 5-hydroxy, 5-substituted-pyrimidine-2,4,6-triones as potent inhibitors of gelatinases MMP-2 and MMP-9.** *Eur. J. Med. Chem.* **2012**, 58, 368-376.

34) Catto M, Berezin AA, Lo Re D, Loizou G, Demetriades M, De Stradis A, Campagna F, Koutentis PA, Carotti A; **Design, synthesis and biological evaluation of benzo[*e*][1,2,4]triazin-7(1*H*)-one and [1,2,4]-triazino[5,6,1-*jk*]carbazol-6-one derivatives as dual inhibitors of beta-amyloid aggregation and acetyl/butyryl cholinesterase**. *Eur. J. Med. Chem.* **2012**, 58, 84-97.

35) Catto M,* Pisani L, Leonetti F, Nicolotti O, Pesce P, Stefanachi A, Cellamare S, Carotti A; **Design, synthesis and biological evaluation of coumarin alkylamines as potent and selective dual binding site inhibitors of acetylcholinesterase.** *Bioorg. Med. Chem.* **2013**, 21, 146-152.

36) Pisani L, Barletta M, Soto-Otero R, Nicolotti O, Mendez-Alvarez E, Catto M, Introcaso A, Stefanachi A, Cellamare S, Altomare C, Carotti A; **Discovery, Biological Evaluation and Structure–Activity and –Selectivity Relationships of 6'-Substituted-(*E*)-2-(benzofuran-3(2*H*)-ylidene)-*N*-methylacetamides, a Novel Class of Potent and Selective Monoamine Oxidase Inhibitors.** *J. Med. Chem.* **2013**, 56, 2651-2664.

37) Pisani L, Catto M, Nicolotti O, Grossi G, Di Braccio M, Soto-Otero R, Mendez-Alvarez E, Stefanachi A, Gadaleta G, Carotti A; **Fine Molecular Tuning at Position 4 of 2H-Chromen-2-one Derivatives in the Search of Potent and Selective Monoamine Oxidase B Inhibitors.** *Eur. J. Med. Chem.* **2013**, 70, 723-739.

38) Catto M, Arnesano F, Palazzo G, De Stradis A, Calò V, Losacco M, Purgatorio R, Campagna F; **Investigation on the influence of (*Z*)-3-(2-(3-chlorophenyl)hydrazono)-5,6-dihydroxyindolin-2-one (PT2) on β-amyloid(1-40) aggregation and toxicity.** *Archiv. Biochem. Biophys.* **2014**, 560, 73-82.

39) Mariano M, Schmitt C, Miralinaghi P, Catto M, Hartmann RW, Carotti A, Engel M; **First selective dual inhibitors of tau phosphorylation and beta-amyloid aggregation, two major pathogenic mechanisms in Alzheimer's disease.** *ACS Chem. Neurosci.*, **2014**, 5, 1198–1202.

40) Pisani L, Farina R, Nicolotti O, Gadaleta D, Soto-Otero R, Catto M, Di Braccio M, Mendez-Alvarez E, Carotti A; **In Silico Design of Novel 2*H*-Chromen-2-one Derivatives as Potent and Selective MAO-B Inhibitors**. *Eur. J. Med. Chem.* **2015**, 89, 98-105.

41) Stefanachi A, Hanke N, Pisani L, Leonetti F, Nicolotti O, Catto M, Cellamare S, Hartmann RW, Carotti A; **Discovery of New 7-Substituted-4-imidazolylmethyl Coumarins and 4'-Substituted-2-Imidazolyl**

**Acetophenones Open Analogues as Potent and Selective Inhibitors of Steroid-11β-hydroxylase**. *Eur. J. Med. Chem.* **2015**, 89, 106-114.

42) Dominguez JL, Fernández-Nieto F, Castro M, Catto M, Paleo MR, Porto S, Sardina FJ, Brea J, Carotti A, Villaverde MC, Sussman FS; **Computer Aided Structure Based Design of Multitarget Leads for Alzheimer's Disease**. *J. Chem. Inf. Model.* **2015**, 55, 135-148.

43) Tonelli M, Catto M,* Tasso B, Novelli F, Canu C, Iusco G, Pisani L, De Stradis A, Denora N, Sparatore A, Boido V, Carotti A, Sparatore F; **Multitarget Therapeutic Leads for Alzheimer's Disease: Quinolizidinyl Derivatives of Bi- and Tri-cyclic Systems as Dual Inhibitors of Cholinesterases and Aβ Aggregation**. *ChemMedChem* **2015**, 10, 1040-1053.

44) Pau A, Catto M,* Pinna G, Frau S, Murineddu G, Asproni B, Curzu MM, Pisani L, Leonetti F, Loza MI, Brea J, Pinna GA, Carotti A; **Multitarget-Directed Tricyclic Pyridazinones as G Protein-Coupled Receptor Ligands and Cholinesterase Inhibitors**. *ChemMedChem* **2015**, 10, 1054-1070.

45) Farina R, Pisani L, Catto M,* Nicolotti O, Gadaleta D, Denora N, Soto-Otero R, Mendez-Alvarez E, Passos CS, Muncipinto G, Altomare CD, Nurisso A, Carrupt PA, Carotti A; **Structure-Based Design and Optimization of Multitarget-Directed 2H- Chromen-2-one Derivatives as Potent Inhibitors of Monoamine Oxidase B and Cholinesterases**. *J. Med. Chem.* **2015**, 58, 5561-5578.

46) Trisciuzzi D, Alberga D, Mansouri K, Judson R, Cellamare S, Catto M, Carotti A, Benfenati E, Novellino E, Mangiatordi GF, Nicolotti O; **Docking-based classification models for exploratory toxicology studies on high-quality estrogenic experimental data.** *Future Med. Chem.* **2015**, 7, 1921-1936.

47) Gadaleta D, Mangiatordi GF, Catto M, Carotti A, Nicolotti O; **Applicability Domain for QSAR models: where theory meets reality.** *IJQSPR* **2016**, 1, 45-63.

48) Pisani L, Farina R, Soto-Otero R, Denora N, Mangiatordi GF, Nicolotti O, Mendez-Alvarez E, Altomare CD, Catto M,* Carotti A; **Searching for Multitargeting Neurotherapeutics against Alzheimer's: Discovery of Potent AChE−MAO B Inhibitors through the Decoration of 2*H*-Chromen-2-one Structural Motif.** *Molecules* **2016**, 21, 362.

49) Mangiatordi GF, Alberga D, Altomare CD, Carotti A, Catto M, Cellamare S, Gadaleta D, Lattanzi G, Leonetti F, Pisani L, Stefanachi A, Trisciuzzi D, Nicolotti O; **Mind the gap! A journey towards computational toxicology**. *Mol. Inf.*, **2016**, 35, 294-308.

50) Domínguez JL, Fernández-Nieto F, Brea JM, Catto M, Paleo MR, Porto S, Sardina FJ, Castro M, Pisani L, Carotti A, Soto-Otero R, Méndez-Alvarez E, M. Villaverde C, Sussman F; **8-Aminomethyl-7-hydroxy-4-methylcoumarins as Multitarget Leads for Alzheimer's Disease**. *ChemistrySelect* **2016**, 1, 2742-2749.

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